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Effects of Rh coordination and surface strain on NO dissociation STEFANO DE GIRONCOLI, PUSHPA RAGHANI, SISSA, Trieste, Italy, PRASENJIT GHOSH, SHOBHANA NARASIMHAN, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India — The Rh(100) surface is known to be a good catalyst for the reduction of NO. We try to understand the effect of Rh coordination and in plane strain on NO adsorption and its dissociation. To distinguish between the strain effects and charge transfer we look at the adsorption and dissociation of NO on Rh(100) and stretched Rh(100), in addition to NO adsorption on 1 ML of Rh/MgO at MgO and Rh lattice constants. As expected, we find that the adsorption energy of NO increases with reduction in effective coordination of Rh, i.e., while going from Rh(100), to stretched Rh(100), to 1 ML Rh/MgO, to 0.25 ML of Rh/MgO. In the case of NO on Rh(100) and on 1 ML Rh/MgO at Rh lattice constant, we find that NO adsorbs vertically at the bridge site between two Rh atoms; whereas, in the case of stretched Rh(100) and 1 ML of Rh/MgO at MgO lattice constant, NO adsorbs horizontally at the hollow site. Hence, as the effective Rh coordination is changed, both adsorption geometries and adsorption energies change in a systematic way. This has an influence on the energetic barriers for the rate-limiting step in the reduciton of NO on these surfaces.

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